Digital Twin of Groundwater: Interactive Modelling of Depletion Dynamics and Trace Metal Mobilization in Aquifers

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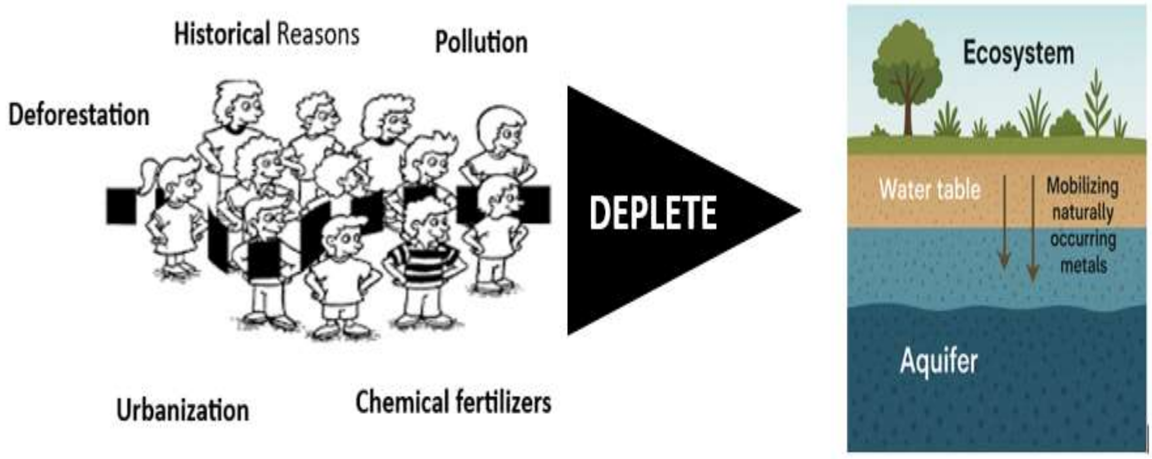
Abstract

Groundwater represents the largest accessible freshwater resource on Earth, playing a critical role in sustaining agriculture, ecosystems, and human livelihoods. However, excessive withdrawal—particularly for irrigation in arid and semi-arid regions—has led to widespread groundwater depletion. This depletion not only reduces water availability but also triggers significant changes in groundwater geochemistry, which can degrade water quality and disrupt dependent ecosystems. As water tables decline, hydrogeochemical interactions between groundwater and aquifer materials intensify, mobilizing naturally occurring contaminants such as arsenic, fluoride, and iron. Furthermore, increased concentrations of total dissolved solids (TDS), salinity, and hardness often result from reduced dilution and prolonged water-rock interaction. Anthropogenic inputs, including agricultural fertilizers and industrial pollutants, further compound chemical degradation. These geochemical shifts can render groundwater unsuitable for drinking and irrigation, posing serious threats to food security, public health, and environmental sustainability. Addressing groundwater depletion thus requires an integrated approach that combines hydrogeological understanding with geochemical monitoring, policy reform, and community-based water management. This highlights the complex interplay between groundwater quantity and quality, emphasizing the need for geochemistry-informed strategies to ensure long-term groundwater sustainability in the face of growing demand and climate variability.

Keywords: Depletion, Geochemistry, Hydrogeochemical interaction, Anthropogenic pollution

Graphical Abstract

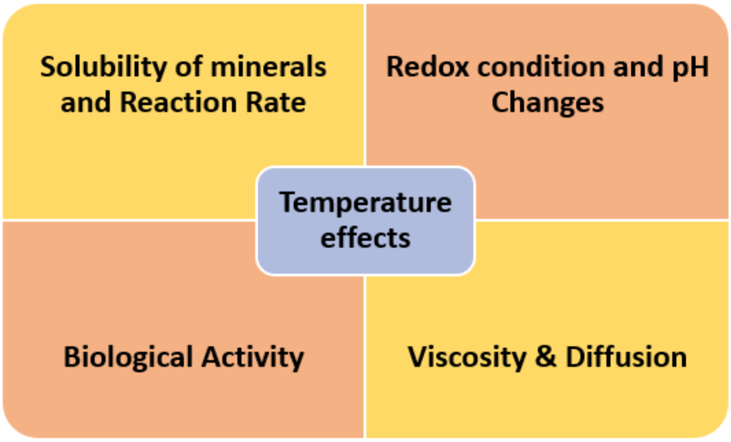


Introduction

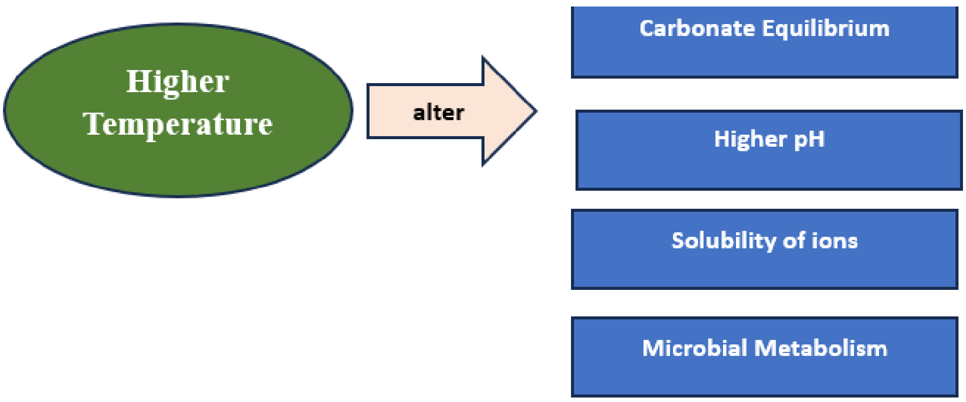
Groundwater, one of the planet's most vital natural resources, plays a crucial role in sustaining agricultural production, supplying drinking water, and supporting ecosystems worldwide. It accounts for approximately one-third of global freshwater withdrawals, with usage rising significantly due to population growth, industrialization, and expanding agricultural demands. However, the overexploitation of aquifers and unsustainable groundwater management practices have led to alarming rates of depletion in many regions. It is stored in the tiny open spaces between rock and sand, soil, and gravel. How well loosely arranged rock holds water depends on the size of the rock particles. Layers of loosely arranged particles of uniform size tend to hold more water than layers of rock with materials of different sizes. The composition of groundwater does not change naturally if there is change recognised in taste, odour and texture it may happened due to the contamination of aquifer. In an aquifer, there is enough groundwater that it can be pumped to the surface and used for drinking water, irrigation, industry, or other uses. *(Todd, D.K., & Mays, L.W. (2005).* The chemical nature of groundwater can be defined on the basis of **temperature, pH, oxidation and reduction potential.** Due to variation in temperature, the level of water table gets disturb as a result recharge rate and chemical state varies, ultimately the composition of groundwater gets changed. *(Vinuta M. Betageri and Rahul Patil; 2010).* A detailed geochemical study of groundwater is used to understand the role of various elements in groundwater aquifer, including all the major ions such as Na, K, Ca, Mg, Fe, Mn, Zn, Cu, Pb, As, Cd and how the elemental fluxes are exchanged through atmospheric, terrestrial and aquatic interactions (Gupta et al., 2009).The cases of poor water quality, decreasing population and life span of aquatic organism, water table instability reported frequently. Chemical characteristics and geochemical process is important to understand the chemical evolution of water that flows through the surface. The presence of the heavy metals in water resources like groundwater is a significant public health concern as well as environmental concern. These heavy metals can accumulate in waterbodies through various sources including industrial discharge, improper waste disposal.

Effect of Temperature

Temperature significantly influences **groundwater chemistry** through a variety of physical, chemical, and biological processes.



Higher temperature leads to increase the solubility of some minerals especially carbonates and silicates. However, some gases like CO_2 and O_2 become less soluble at higher temperature which leads to reduce in groundwater. Chemical reaction accelerates on increasing temperature. Temperature can shift **oxidation-reduction (redox) balance**: Warmer conditions can enhance microbial **decomposition of organic matter**, consuming O_2 and potentially leading to **reducing conditions**. This can mobilize elements like **Fe, Mn, As, and U**, which are more soluble in reduced states.

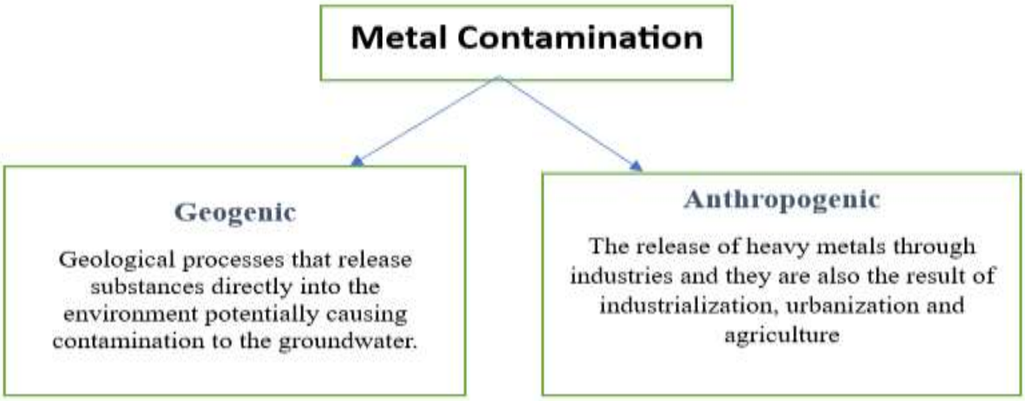


Factors Affecting Microbial Metabolism
Denitrification
Sulfate Reduction
Methanogenesis

Temperature influences how metals bind to soil or sediment particles. Higher temperatures can reduce adsorption and increase desorption, releasing more metals into groundwater.

Metallurgy of Groundwater

In India, The metallurgy of groundwater generally refers to the metal content present or contamination in groundwater and how these metals interact with the natural environment. The presence of the heavy metals in water resources like groundwater is a serious public health concern as well as environmental problem. These heavy metals can accumulate in waterbodies through various sources including industrial discharge, improper waste disposal. (Kumar et al., 2014).



ESSENTIAL METALS	TOXIC/ HEAVY METALS
Iron (Fe)	Arsenic (As)
Manganese (Mn)	Lead (Pb)
Zinc (Zn)	Cadmium (Cd)
Copper (Cu)	Chromium (Cr)
Selenium (Se)	Mercury (Hg)
Molybdenum (Mo)	Aluminium (Al)

Health impact on Humans

Heavy metals present in drinking groundwater can lead to the serious health problems when they were consumed for a long duration of time. Exposure of Lead is directly linked to the neurological disorders, especially in children, by affecting their cognitive skills and behaviour. Cadmium is associated to the kidney damage and bone fractures. Chronic exposure to the Mercury impairs the nervous system of the humans which leads to the symptoms such as memory loss, motos dysfunction etc. Similarly, long-term exposure to the Arsenic is known to cause skin lesions, respiratory issue and various types of cancers. *(Source: WHO, 2017; Sharma & Wadhvani, 2015)*

METALS	SOURCES	HEALTH EFFECTS
ARSENIC(As)	Rocks and industrial waste	**It causes cancer, skin lesions and developmental effects**
LEAD (Pb)	Old plumbing and battery waste	**It causes neurological damage especially in children**
CADMIUM (Cd)	Fertilizers and industrial run off	**It causes kidney damage and bone weakness**
IRON (Fe)	Naturally from rocks	**It causes staining, metallic taste which is not very toxic**
MANGANESE (Mn)	Natural and industrial processes	**It causes neurological effects at high levels**
CHROMIUM (Cr)	From electroplating industries	**It causes carcinogenic and respiratory problems**
ZINC (Zn)	From industrial waste and galvanized pipes	**It causes nausea, stomach ache when consumed in high dose**
FLUORIDE (F)	Weathering of fluoride rich minerals	**It causes dental and skeletal fluorosis**

Ecological Effect

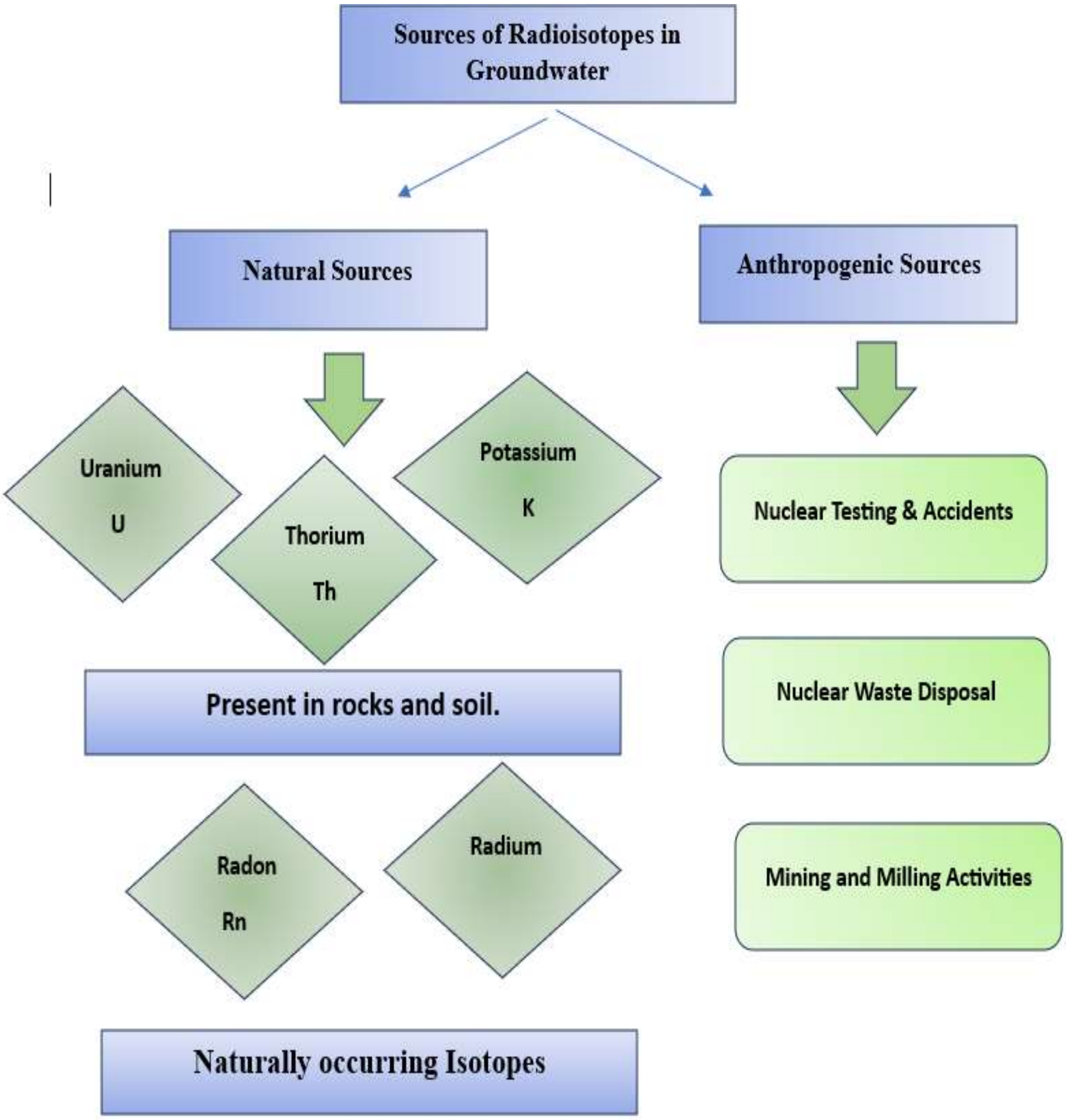
The presence of heavy metals in groundwater also has adverse effect on aquatic ecosystems. These can accumulate in sediments which afterwards enter the aquatic food chain leading to bioaccumulation and biomagnification. *(Ali et al., 2019)* The elevated levels of metals like Chromium and Nickel, they are specially known to reduce biodiversity by affecting the reproductive and survival rates of sensitive species.

Economic and Social Consequences

Heavy metals contamination in groundwater impacts both economy and society. The polluted groundwater limit access to safe drinking water, which increase the need of costly water supply and purification process throughout the affected region. The loss of biodiversity and ecosystem service due to heavy and toxic metals also disrupts tourism and recreational activities in affected region. *(Foster & Chilton, 2003)*

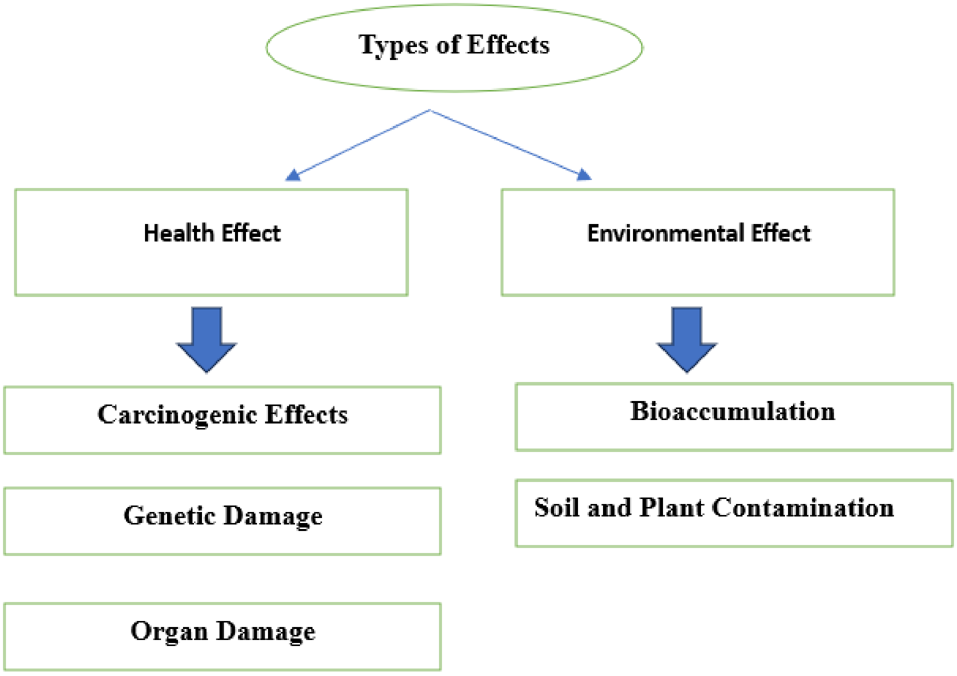
Radiology of Groundwater

Radioisotopes, in groundwater pose significant environmental and public health concerns. These isotopes may be naturally occurring or introduced through anthropogenic (human-related) activities. Understanding their sources, behaviour in the subsurface environment, and potential risks is essential for water safety and public health management. (*IAEA, 2010)*



Harmful impact of Radioisotopes on groundwater

Ingestion or inhalation of radioactive water or gases (like radon) can lead to cancer, especially of the lungs, bones, and kidneys are considered as carcinogenic effects whereas Long-term exposure can cause DNA damage and reproductive effects are genetic damage. Accumulated radiation doses may impair organs such as the kidneys and liver are organ damage. Radioisotopes can concentrate in aquatic food chains at different tropic levels is considered as bioaccumulation. Irrigation with contaminated groundwater can transfer isotopes into crops leads to soil and plant contamination.



Conclusion

Groundwater, a vital freshwater resource, is under threat from overexploitation, particularly in arid regions. Depletion alters geochemical interactions, leading to the mobilization of harmful elements like arsenic, fluoride, and heavy metals. Elevated temperatures, industrial discharge, and agricultural activities further degrade water quality, affecting human health, ecosystems, and economic stability. Radioisotope contamination poses additional long-term risks through bioaccumulation and genetic damage. Addressing these issues requires integrated strategies combining hydrogeological insight, geochemical monitoring, policy reform, and community participation. Ensuring groundwater sustainability amid climate variability and rising demand is essential for protecting public health, preserving ecosystems, and securing long-term water resources.

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